

=> s 16

L7 15 L6

=> d abs fbib hitstr 1-15

L7 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

AB A novel, bis(peptide) based mol. actuator has been synthesized. It is demonstrated to undergo contraction and expansion controlled by the addition and removal of Cu<sup>2+</sup>; this is demonstrated by the direct observation of a change in hydrodynamic properties by using sedimentation anal. and size exclusion chromatog. The mol. undergoes a large change in sedimentation coefficient, axial ratio, and size exclusion chromatog. elution time when it binds copper. The demonstration of the bis(peptide)-based mech. mol. actuator controlled change in the mech. properties of make it a good starting point for the development of mol. devices that will harness changes in mol. shape and size to create mol. devices such as sensors or valves.

AN 2008:963220 CAPLUS

TI Observation of contraction and expansion in a bis(peptide)-based mechanical molecular actuator

AU Schafmeister, Christian E.; Belasco, Laura G.; Brown, Patrick H.

CS Department of Chemistry, Temple University, Philadelphia, PA, 19122, USA

SO Chemistry--A European Journal (2008), 14(21), 6406-6412

CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

IT 1063588-57-7D, copper complexes

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)

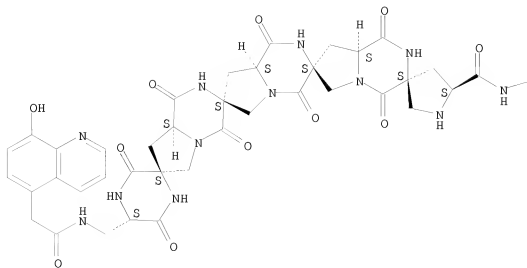
(solid phase peptide synthesis and contraction and expansion in bispeptide-based mech. mol. actuator)

RN 1063588-57-7 CAPLUS

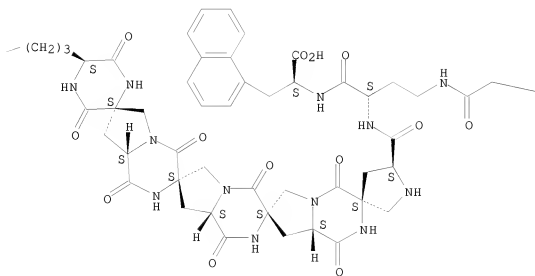
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

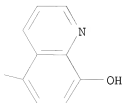
PAGE 1-A



PAGE 1-B



PAGE 1-C



RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(solid phase peptide synthesis and contraction and expansion in bispeptide-based mech. mol. actuator

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2008 ACS ON STN  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The authors have developed second-generation monomers I (n = 1, 2) and improved conditions for rapidly and simultaneously closing multiple diketopiperazines on solid support. These new conditions involve either the microwave heating of a suspension of solid-supported amino-tetrafluoropropyl esters in acetic acid/triethylamine catalyst solution or continuous flow of catalyst solution through the resin, heated in a flow cell apparatus. The authors demonstrate that monomers I and II can be combined with the new conditions easily to synthesize previously inaccessible hetero and homo spiro ladder oligomers III and IV.

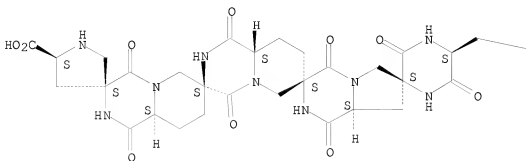
AN 2006:1084746 CAPLUS  
DN 146:63073  
TI Synthesis of structurally diverse bis-peptide oligomers  
AU Gupta, Sharad; Macala, Megan; Schafmeister, Christian E.  
CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA  
SO Journal of Organic Chemistry (2006), 71(23), 8691-8695  
CODEN: JOCEAH; ISSN: 0022-3263  
PB American Chemical Society  
DT Journal  
LA English  
OS CASREACT 146:63073  
IT 916987-06-9DP, resin-bound 916987-07-0DP, resin-bound  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of (carboxy)(amino)prolines and (carboxy)(amino)pipecolic acids for synthesis of spiro ladder oligomers via diketopiperazine formation)

RN 916987-06-9 CAPLUS  
CN Tetraspiro[piperazine-2,7' (6'H)-pyrrolo[1,2-a]pyrazine-3' (4'H),7'' (6' 'H)-

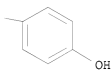
[2H]pyrido[1,2-a]pyrazine-3'''(4''H),7'''(6'''H)-[2H]pyrido[1,2-a]pyrazine-3'''(4'''H),3'''-pyrrolidine]-5'''-carboxylic acid, dodecahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',1''',3,4',4'',4''',6-octaoxo-, (2S,3'S,3'''S,3''''S,5S,5''''S,8'aS,9''aS,9'''aS)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

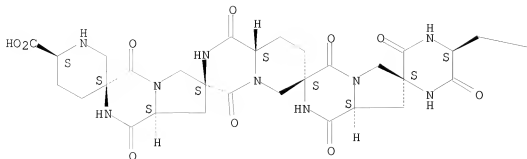


RN 916987-07-0 CAPLUS

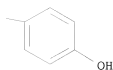
CN Tetraspiro[piperazine-2,7'(6'H)-pyrrolo[1,2-a]pyrazine-3'(4'H),7''(6''H)-[2H]pyrido[1,2-a]pyrazine-3'''(4''H),7'''(6'''H)-pyrrolo[1,2-a]pyrazine-3'''(4'''H),3'''-piperidine]-6'''-carboxylic acid, dodecahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',1''',3,4',4'',4''',6-octaoxo-, (2S,3'S,3'''S,3''''S,5S,6''''S,8'aS,8''aS,9''aS)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

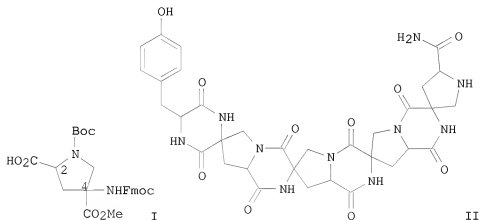


PAGE 1-B



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



AB Using trans-4-hydroxy-L-proline as a precursor, all stereoisomers of 1-Boc-4-(Fmoc-amino)-4-(methoxycarbonyl)proline I [(2S,4R), (2R,4S), (2S,4S), (2R,4R); Boc = tert-butoxycarbonyl; Fmoc = 9-fluorenylmethoxycarbonyl] as monomers were prepared. This small library of monomers allowed arbitrary stereochem. configuration at any chiral center.

within spiro-ladder oligomers II. Three tetramer oligomers containing several combinations of I were synthesized. The effect of monomer sequence on scaffold conformation by NMR was examined

AN 2006:483262 CAPLUS

DN 145:167507

TI Maximizing the Stereochemical Diversity of Spiro-Ladder Oligomers

AU Levine, Christopher G.; Brown, Zachary Z.; Schafmeister, Christian E.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO Organic Letters (2006), 8(13), 2807-2810

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 145:167507

IT 900149-01-1P 900149-02-2P 900149-03-3P

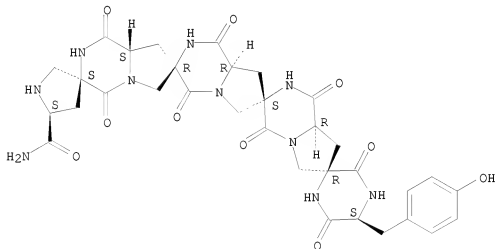
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and conformations of stereochem. spiro-ladder oligomers derived from (amino) (carboxy)proline monomers)

RN 900149-01-1 CAPLUS

CN Tetraspiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3''(4'H),7'''(6''H)-pyrrolo[1,2-a]pyrazine-3'''(4'''H),7''''(6'''H)-pyrrolo[1,2-a]pyrazine-3''''(4''''H),3''''-pyrrolidine]-5''''-carboxamide, dodecahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',1''',3,4',4'',4''',6-octaoxo-, (2R,3'R,3''R,3'''S,5S,5''S,5'''S,8'aR,8''aR,8'''aS)- (9CI) (CA INDEX NAME)

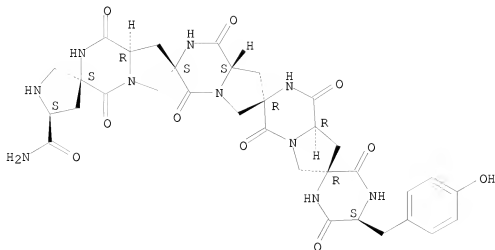
Absolute stereochemistry.



RN 900149-02-2 CAPLUS

CN Tetraspiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3''(4'H),7'''(6''H)-pyrrolo[1,2-a]pyrazine-3'''(4'''H),7''''(6'''H)-pyrrolo[1,2-a]pyrazine-3''''(4''''H),3''''-pyrrolidine]-5''''-carboxamide, dodecahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',1''',3,4',4'',4''',6-octaoxo-, (2R,3'R,3''S,3'''S,5S,5''S,5'''S,8'aR,8''aS,8'''aR)- (9CI) (CA INDEX NAME)

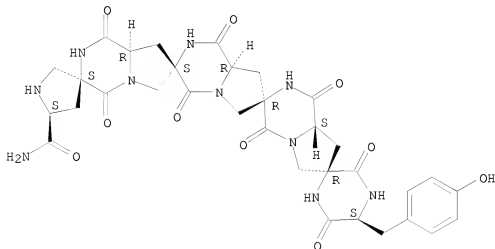
Absolute stereochemistry.



RN 900149-03-3 CAPLUS

CN Tetraspiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3'-(4'H),7''-(6''H)-pyrrolo[1,2-a]pyrazine-3'''-(4'''H),7''''-(6''''H)-pyrrolo[1,2-a]pyrazine-3''''-(4''''H),3'''''-pyrrolidine]-5''''-carboxamide, dodecahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',1''',3,4',4'',4''',6-octaoxo-, (2R,3'R,3'''S,3''''S,5S,5''''S,8'aS,8''aR,8'''aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 900148-98-3P 900148-99-4P 900149-00-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

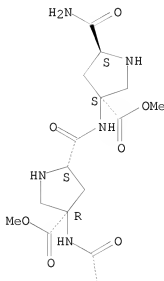
(preparation and conformations of stereochem. spiro-ladder oligomers derived from (amino)(carboxy)proline monomers)

RN 900148-98-3 CAPLUS

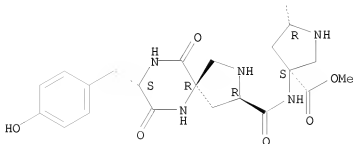
CN 3-Pyrrolidinecarboxylic acid, 5-[[[(3S,5S)-5-(aminocarbonyl)-3-(methoxycarbonyl)-3-pyrrolidinyl]amino]carbonyl]-3-[[[(2R,4S)-4-[[[(3R,5R,8S)-8-[(4-hydroxyphenyl)methyl]-7,10-dioxo-2,6,9-triazaspiro[4.5]dec-3-yl]carbonyl]amino]-4-(methoxycarbonyl)-2-pyrrolidinyl]carbonyl]amino]-, methyl ester, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



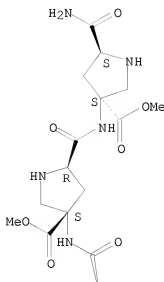
RN 900148-99-4 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 5-[[[(3S,5S)-5-(aminocarbonyl)-3-

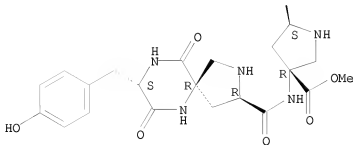
(methoxycarbonyl)-3-pyrrolidinyl]amino]carbonyl]-3-[[[(2S,4R)-4-[[[(3R,5R,8S)-8-[(4-hydroxyphenyl)methyl]-7,10-dioxo-2,6,9-triazaspiro[4.5]dec-3-yl]carbonyl]amino]-4-(methoxycarbonyl)-2-pyrrolidinyl]carbonyl]amino]-, methyl ester, (3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



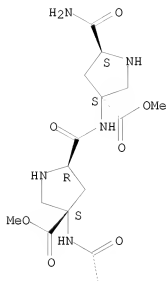
RN 900149-00-0 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 5-[[[(3S,5S)-5-(aminocarbonyl)-3-(methoxycarbonyl)-3-pyrrolidinyl]amino]carbonyl]-3-[[[(2R,4R)-4-[[[(3S,5R,8S)-8-[(4-hydroxyphenyl)methyl]-7,10-dioxo-2,6,9-triazaspiro[4.5]dec-3-yl]carbonyl]amino]-4-(methoxycarbonyl)-2-pyrrolidinyl]carbonyl]amino]-, methyl ester, (3S,5R)- (9CI) (CA INDEX

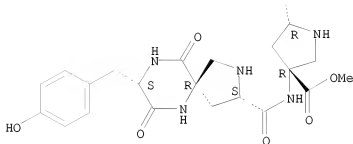
NAME)

Absolute stereochemistry.

PAGE 1-A

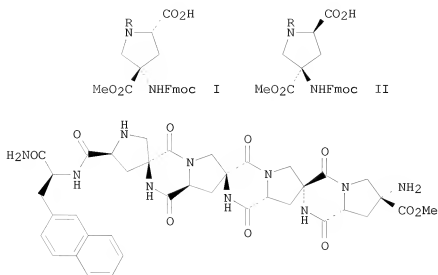


PAGE 2-A



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



III

AB Spiro-ladder oligomers of designed shape were assembled from a set of two enantiomeric bis-amino acid monomers I and II (R = Cbz, Boc). Two tetramers of differing monomer sequence were synthesized to study the effect of monomer stereochem. upon macromol. shape. For example, using protected 4-amino-4-carboxyprolines I, II (R = Cbz), Fmoc-(S)-2-naphthylalanine and solid-phase peptide synthesis methods, spiro-ladder tetramer III was synthesized. Two-dimensional NMR expts. were used to determine the conformational preference of the monomers within the context of the oligomers. The results of this structural study were used to design two pentamers: one resembling a rod and another with a curved shape. The pentamers were end-labeled with naphthyl and dansyl groups. The design hypothesis was confirmed by measuring the efficiency of fluorescence resonance energy transfer between the naphthyl and dansyl fluorophore pair.

AN 2005:1062317 CAPLUS

DN 144:7065

TI The Synthesis of Curved and Linear Structures from a Minimal Set of Monomers

AU Levins, Christopher G.; Schafmeister, Christian E.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO Journal of Organic Chemistry (2005), 70(22), 9002-9008

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 144:7065

IT 870097-42-0P

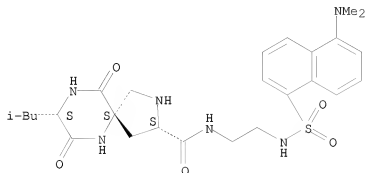
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (control compound; preparation and conformations of spiro-ladder oligomers derived from (amino)(carboxy)proline monomers)

RN 870097-42-0 CAPLUS

CN 2,6,9-Triazaspiro[4.5]decane-3-carboxamide, N-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]-8-(2-

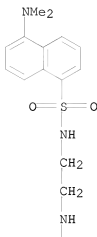
methylpropyl)-7,10-dioxo-, (3S,5S,8S)- (CA INDEX NAME)

Absolute stereochemistry.

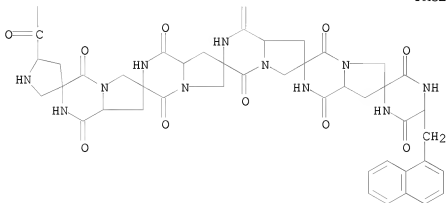


IT 870097-38-4P 870097-40-8P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and conformations of spiro-ladder oligomers derived from  
 (amino) (carboxy) proline monomers)  
 RN 870097-38-4 CAPLUS  
 CN Pentaspiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3''(4'H),7'''(6''H)-  
 pyrrolo[1,2-a]pyrazine-3'''(4''H),7''''(6''''H)-pyrrolo[1,2-a]pyrazine-  
 3''''(4''''H),7'''''(6'''''H)-pyrrolo[1,2-a]pyrazine-3'''''(4'''''H),3''''''-  
 pyrrolidine]-5''''''-carboxamide, N-[2-[[5-(dimethylamino)-1-  
 naphthalenyl]sulfonyl]amino]ethyl]hexadecahydro-5-(1-naphthalenylmethyl)-  
 1'',1''',1''''',1'''''',3,4'',4''',4''''',4''''''',6-decaoxo-,  
 (2S,3'S,3''S,3'''S,3''''S,3'''''S,5S,5''S,5'''S,5''''S,8'aS,8''aS,8'''aS,8''''aS)- (9CI)  
 (CA INDEX NAME)

PAGE 1-A



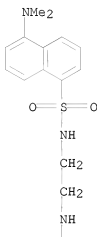
PAGE 2-A



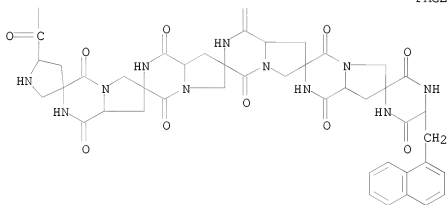
RN 870097-40-8 CAPLUS

CN Pentaspiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3''(4'H),7'''(6'''H)-pyrrolo[1,2-a]pyrazine-3'''(4'''H),7''''(6''''H)-pyrrolo[1,2-a]pyrazine-3''''(4''''H),3''''-(4''''H)-pyrrolo[1,2-a]pyrazine-3''''(4''''H),3''''-(4''''H)-pyrrolidine]-5''''-carboxamide, N-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]hexadecahydro-5-(1-naphthalenylmethyl)-1',1'',1''',1''''(3,4',4'',4''',4''''(6-decaoxo-, (2S,3'R,3''S,3''''R,3''''''S,5S,5''''''S,8'aS,8''aR,8''''aS,8''''''aR)- (9CI)  
(CA INDEX NAME)

PAGE 1-A

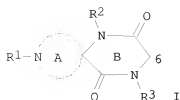


PAGE 2-A



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



AB The title compds. I [ring A = (un)substituted 3 to 15-membered N-containing monocyclic, dicyclic, or tricyclic heterocyclic ring; ring B may have a substituent [e.g., (un)substituted aliphatic hydrocarbon group, etc.] at position 6; R1 = H, (un)substituted aliphatic hydrocarbon group, etc.; R2, R3 = H, aliphatic hydrocarbon group, etc.] are prepared. Thus, 2-morpholinoethyl isocyanide was added to a mixture of 1-benzyl-3-methyl-4-piperidone, (2S)-2-(tert-butoxycarbonylamino)-3-cyclohexylpropanoic acid, and butylamine in methanol; the resulting mixture was stirred overnight at 50°C; after cooling, HCl was added to the reaction mixture, and said mixture was stirred for 2 h at 60°C; the reaction mixture was worked up and extracted with dichloromethane; the extract was concentrated; 1.25 M acetic acid

solution in toluene was added to the concentrate; the resulting mixture was stirred overnight at 100°C to give, after purification and treatment with HCl, (3S)-9-benzyl-1-butyl-3-(cyclohexylmethyl)-7-methyl-1,4,9-triazaspiro[5.5]undecane-2,5-dione hydrochloride (II). In an in vitro assay for human CCR5 receptor antagonism, II showed IC50 value of 0.76 µM. The compds. represented by the general formula I are said to be useful in preventing and/or treating various diseases such as acquired immune deficiency syndrome, etc. Formulations are given.

AN 2004:927209 CAPLUS

DN 141:395575

TI Preparation of triazaspiroalkanedione derivatives as chemokine receptor antagonists

IN Nishizawa, Rena; Takaoka, Yoshikazu; Shibayama, Shiro

PA Ono Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 78 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

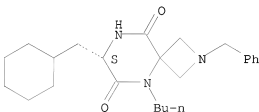
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004094424	A1	20041104	WO 2004-JP5610	20040420
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,				
	TD, TG				

EP 1621540 A1 20060201 JP 2003-116235 A 20030421  
 EP 2004-728443 20040420  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK  
 JP 2003-116235 A 20030421  
 WO 2004-JP5610 W 20040420  
 US 20070155713 A1 20070705 US 2005-554096 20051021  
 JP 2003-116235 A 20030421  
 WO 2004-JP5610 W 20040420

OS MARPAT 141:395575  
 IT 787629-01-0P 787629-02-1P 787629-03-2P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (preparation of triazaspiroalkanedione derivs. as chemokine receptor  
 antagonists)

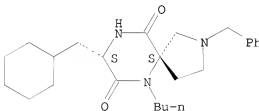
RN 787629-01-0 CAPLUS  
 CN 2,5,8-Triazaspiro[3.5]nonane-6,9-dione,  
 5-butyl-7-(cyclohexylmethyl)-2-(phenylmethyl)-, (7S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 787629-02-1 CAPLUS  
 CN 2,6,9-Triazaspiro[4.5]decane-7,10-dione,  
 6-butyl-8-(cyclohexylmethyl)-2-(phenylmethyl)-, hydrochloride (1:1),  
 (5S,8S)- (CA INDEX NAME)

Absolute stereochemistry.

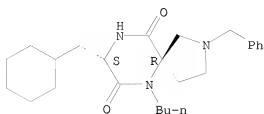


● HCl

RN 787629-03-2 CAPLUS  
 CN 2,6,9-Triazaspiro[4.5]decane-7,10-dione,  
 6-butyl-8-(cyclohexylmethyl)-2-(phenylmethyl)-, hydrochloride (1:1),

(5R,8S)- (CA INDEX NAME)

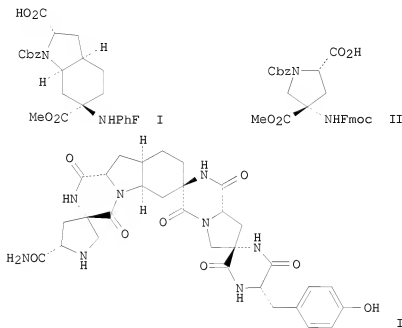
Absolute stereochemistry.



● HCl

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



AB The synthesis of a new bis-amino acid, amino(perhydroindole)dicarboxylate I (PhF = 9-phenylfluoren-9-yl), is presented. I was designed to create a tightly curved structure when assembled into oligomers. I was coupled

with proline derivative II to afford a strongly bent spiro-ladder oligomer III. The structure of III was determined in aqueous solution using two-dimensional

NMR.

AN 2004:678951 CAPLUS

DN 141:332441

TI Synthesis of a bis-amino acid that creates a sharp turn

AU Habay, Stephen A.; Schafmeister, Christian E.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO Organic Letters (2004), 6(19), 3369-3371

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 141:332441

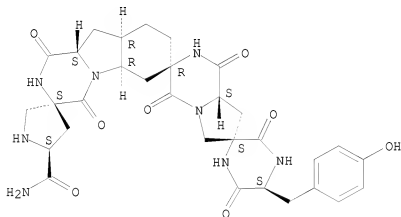
IT 773894-69-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of bis-amino acid amino(perhydroindole)dicarboxylate and its incorporation into diketopiperazine-based oligomer with sharp turn conformation)

RN 773894-69-2 CAPLUS

CN Trispiropiperazine-2,7'(6'H)-pyrrolo[1,2-a]pyrazine-3'(4'H),7''(2'H)-pyrazino[1,2-a]indole-3''(4'H),3'''-pyrrolidine]-5'''-carboxamide, dodecahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',4',4'',3,6-hexaaxo-, (2S,3'R,3''S,5S,5'aR,5''S,8'aS,9'aR,10'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 773894-73-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

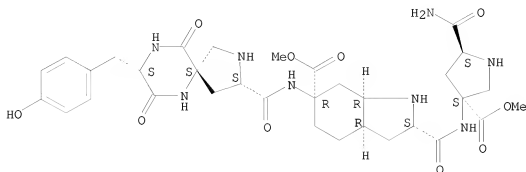
(preparation of bis-amino acid amino(perhydroindole)dicarboxylate and its incorporation into diketopiperazine-based oligomer with sharp turn conformation)

RN 773894-73-8 CAPLUS

CN 1H-Indole-6-carboxylic acid, 2-[[[(3S,5S)-5-(aminocarbonyl)-3-(methoxycarbonyl)-3-pyrrolidinyl]amino]carbonyl]octahydro-6-[[[(3S,5S,8S)-8-[(4-hydroxyphenyl)methyl]-7,10-dioxo-2,6,9-triazaspiro[4.5]dec-3-

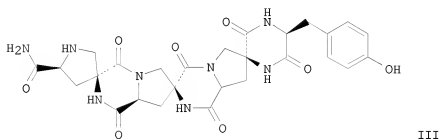
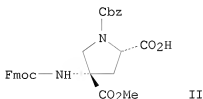
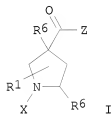
yl]carbonyl]amino]-, methyl ester, (2S,3aR,6R,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



AB The invention provides mol. building blocks of rigid bis(amino acids), which can be linked together through the formation of rigid diketopiperazine rings to provide the desired three dimensional structure. The bis(amino acid) building blocks are applied to the synthesis of macromols. Comps. such as I (R1 is H or a functional group; R5 is N3 or NR2Y, where Y is a protecting group and R2 is H or a functional group; R6 is CO2H or a strongly-activated ester; X is a protecting group; Z is a

weak leaving group) are claimed. Thus, building block II (Cbz = benzyloxycarbonyl, Fmoc = fluorenylmethoxycarbonyl) was prepared from trans-4-hydroxy-L-proline and applied to the sequential solid-phase synthesis of mol. rod III.

AN 2004:120944 CAPLUS

DN 140:181808

TI Preparation of bis(amino acid) molecular scaffolds

IN Schafmeister, Christian E.

PA University of Pittsburgh of the Commonwealth System of Higher Education, USA

SO PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004013282	A2	20040212	WO 2003-US21399	20030705
	WO 2004013282	A3	20040617		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
				US 2002-401474P	P 20020806
				US 2003-612098	A 20030702
				US 2003-613961	A 20030705
	US 20040082783	A1	20040429	US 2003-612098	20030702
				US 2002-401474P	P 20020806
	AU 2003248883	A1	20040223	AU 2003-248883	20030705
				US 2002-401474P	P 20020806
				US 2003-612098	A 20030702
				US 2003-613961	A 20030705
				WO 2003-US21399	W 20030705
	US 20040077879	A1	20040422	US 2003-613961	20030705
				US 2002-401474P	P 20020806
	US 20060217534	A1	20060928	US 2006-432279	20060511
				US 2002-401474P	P 20020806
				US 2003-613961	A3 20030705

OS MARPAT 140:181808

IT 526223-07-4P

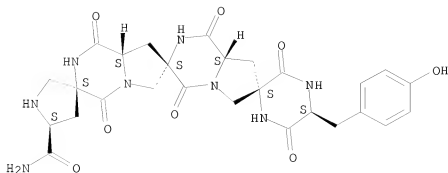
RL: SPN (Synthetic preparation); PREP (Preparation)

(proline bis(amino acid) derivs. in synthesis of piperazinediones)

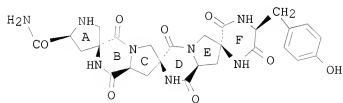
RN 526223-07-4 CAPLUS

CN Tripiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3'-(4'H),7''-(6''H)-pyrrolo[1,2-a]pyrazine-3''-(4''H),3'''-pyrrolidine]-5'''-carboxamide, octahydro-5-[(4-hydroxyphenyl)methyl]-1'',1'',3,4',4'',6-hexaexo-, (2S,3'S,3''S,5S,5''S,8'aS,8''aS)-(9CI) (CA INDEX NAME)

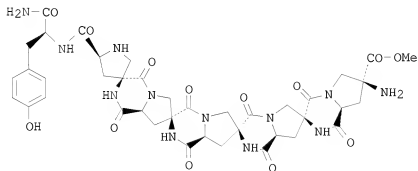
Absolute stereochemistry.



L7 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



I



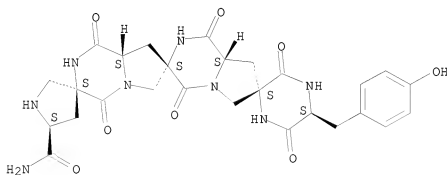
II

AB We report a synthetic approach to spiro-ladder oligomers of defined length and structure that form water-soluble mol. rods. We describe the synthesis of a chiral mol. building block and its assembly on solid support to form flexible chains that were then rigidified by the parallel formation of several diketopiperazine rings. Two mol. rods approx. 15 and 25 Å in length were synthesized containing three and five monomers, resp. (I and II). The mol. rods were easily functionalized on both ends and were shown to have high water solubility, making them compatible with biol. buffers. These mols. may find use as scaffolds for the display of ligands in chemical-biol. applications and as spacers and construction materials for nanoscience applications.

AN 2003:242711 CAPLUS

DN 138:385036  
 TI The Synthesis of Functionalized Nanoscale Molecular Rods of Defined Length  
 AU Levins, Christopher G.; Schafmeister, Christian E.  
 CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260,  
 USA  
 SO Journal of the American Chemical Society (2003), 125(16), 4702-4703  
 CODEN: JACSAT; ISSN: 0002-7863  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 138:385036  
 IT 526223-07-4P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of functionalized nanoscale mol. rods of defined length)  
 RN 526223-07-4 CAPLUS  
 CN Trispiro[piperazine-2,7'-(6'H)-pyrrolo[1,2-a]pyrazine-3'-(4'H),7''-(6''H)-  
 pyrrolo[1,2-a]pyrazine-3'''-(4'''H),3'''-pyrrolidine]-5'''-carboxamide,  
 octahydro-5-[(4-hydroxyphenyl)methyl]-1',1'',3,4',4'',6-hexaaxo-,  
 (2S,3'S,3''S,5S,5'''S,8'aS,8''aS)- (9CI) (CA INDEX NAME)

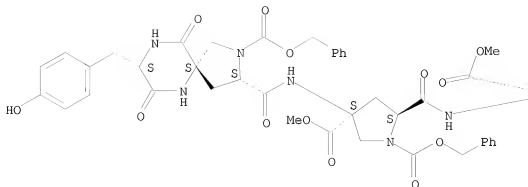
Absolute stereochemistry.



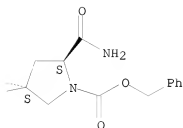
IT 526223-05-2P 526223-06-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (synthesis of functionalized nanoscale mol. rods of defined length)  
 RN 526223-05-2 CAPLUS  
 CN 1,3-Pyrrolidinedicarboxylic acid, 5-(aminocarbonyl)-3-[[[(2S,4S)-4-  
 [[[(3S,5S,8S)-8-[(4-hydroxyphenyl)methyl]-7,10-dioxo-2-  
 [(phenylmethoxy)carbonyl]-2,6,9-triazaspiro[4.5]dec-3-yl]carbonyl]amino]-4-  
 (methoxycarbonyl)-1-[(phenylmethoxy)carbonyl]-2-  
 pyrrolidinyl]carbonyl]amino]-, 3-methyl 1-(phenylmethyl) ester, (3S,5S)-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



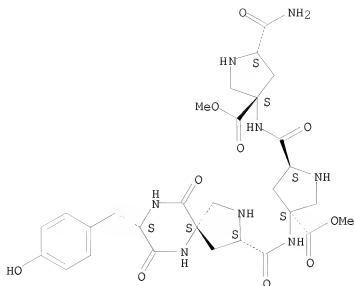
PAGE 1-B



RN 526223-06-3 CAPLUS

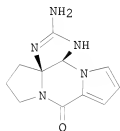
CN 3-Pyrrolidinecarboxylic acid, 5-(aminocarbonyl)-3-[[[(2S,4S)-4-[[[(3S,5S,8S)-8-[(4-hydroxyphenyl)methyl]-7,10-dioxo-2,6,9-triazaspiro[4.5]dec-3-yl]carbonyl]amino]-4-(methoxycarbonyl)-2-pyrrolidinyl]carbonyl]amino]-, methyl ester, (3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

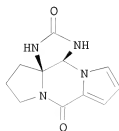


RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



I



II

AB Monoenolates of C2-sym., proline-derived piperazine-2,5-diones were generated and trapped with a variety of electrophiles to produce, in a highly diastereoselective fashion, functionalized diketopiperazines (DKPs). These reactions provide the basis for an asym., desymmetrization strategy toward the marine alkaloids phakellstatin (I) and phakellin (II). The relative stereochem. of the functionalized DKPs was confirmed by single-crystal X-ray anal. and/or NOE expts. Bis-functionalization of the DKPs was also found to proceed with high levels of diastereoselectivity.

AN 2002:525797 CAPLUS  
DN 137:217122

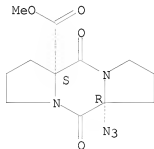
TI Highly Diastereoselective Desymmetrizations of Cyclo(Pro,Pro): An Enantioselective Strategy toward Phakellstatin and Phakellin

AU Poullennec, Karine G.; Kelly, Anna T.; Romo, Daniel

CS Department of Chemistry, Texas A&M University, College Station, TX,

77842-3012, USA  
SO Organic Letters (2002), 4(16), 2645-2648  
CODEN: ORLEF7; ISSN: 1523-7060  
PB American Chemical Society  
DT Journal  
LA English  
OS CASREACT 137:217122  
IT 454693-82-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and hydrogenolysis of; enantioselective strategy toward  
phakellstatin and phakellin via a highly diastereoselective  
desymmetrizations of a chiral proline cyclic dimer)  
RN 454693-82-4 CAPLUS  
CN 1H,5H-Dipyrrolo[1,2-a:1',2'-d]pyrazine-5a(6H)-carboxylic acid,  
10a-azido-hexahydro-5,10-dioxo-, methyl ester, (5aS,10aR)- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

AB The purpose of this study was to identify four major degradation products, which were formed during a stress study of pexiganan (a 22-mer peptide) in a 1% formulation. The degradation products were isolated and characterized by LC/MS, tryptic and aminopeptidase digests. One of the degradation products was shown to be des-Glyl-pexiganan. The other three are structural isomers of N-glyoxylyl-desGlyl-pexiganan. These isomers undergo reversible inter-conversions, as well as decompose irreversibly to des-Glyl-pexiganan. Thus, all the impurities were formed from a single oxidation product of pexiganan, N-glyoxylyl-des-glyl-pexiganan. The aldehyde group of the glyoxylyl residue and the NH-amide of the adjacent isoleucine residue form a piperazinedione derivative of des-glyl-pexiganan. This heterocyclic compound rearranges to other tautomers or back to the N-glyoxylyl compound. Tryptic digests of the three degradation products showed that their N-terminal segment produced N-glyoxylyl-I-G-K whereas the N-terminal segment of pexiganan produced G-I-G-K. All the other tryptic-digest segments were identical to those formed in pexiganan. The LC/MS of the N-terminal segment and of synthetic N-glyoxylyl-I-G-K were identical. The enzymic resistance of the three impurities to undergo aminopeptidase-M cleavage further supported the conclusion that their N-terminal amino residues are substituted. After a year under stress

conditions 1% pexiganan cream lost about 15% of the active component to oxidative-deamination, where the N-terminal glycine residue was oxidized to N-glyoxylyl-des-glyl-pexiganan. The other nine  $\epsilon$ -amino lysine-residues of the peptide stayed intact. This oxidation product inter-converted and formed two addnl. impurities, tautomers of piperazinedionyl-des-Glyl-pexiganan, and decomposed to des-Glyl-pexiganan, the forth impurity.

AN 2000:207984 CAPLUS

DN 133:79160

TI Oxidation of the N-terminal Gly-residue of peptides: stress study of pexiganan acetate in a drug formulation

AU Feibush, Binyamin; Snyder, Bradley C.

CS Magainin Pharmaceuticals, Inc., Plymouth Meeting, PA, 19462, USA

SO Pharmaceutical Research (2000), 17(2), 197-204

CODEN: PHREEB; ISSN: 0724-8741

PB Kluwer Academic/Plenum Publishers

DT Journal

LA English

IT 279216-87-4P

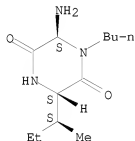
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(oxidation of the N-terminal Gly-residue in stress study of pexiganan acetate in a drug formulation)

RN 279216-87-4 CAPLUS

CN 2,5-Piperazinedione, 6-amino-1-butyl-3-[(1S)-1-methylpropyl]-, (3S,6S)-(CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

AB A synthetic route to a novel  $\alpha,\alpha$ -diamino  $\beta$ -keto ethoxycarbonyl-containing dioxopiperazine, capable of mimicking a  $\beta$ -turn, is reported. The cis configuration of the dioxopiperazine is rationalized by NMR spectroscopy, while computational energy calcs. are used to explain the reluctance to cyclize of N-terminal partially protected dipeptides containing  $\alpha,\alpha$ -diamino groups.

AN 2000:13541 CAPLUS

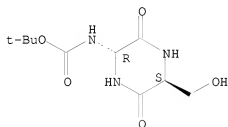
DN 132:308620

TI The synthesis and conformational aspects of a novel dioxopiperazine-a possible  $\beta$ -turn constraint

AU Davies, John S.; Stelmach-Diddams, Malgosia; Fromentin, Regis; Howells,

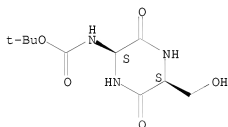
Alun; Cotton, Ron  
 CS Department of Chemistry, University of Wales, Swansea, SA2 8PP, UK  
 SO Perkin 1 (2000), (2), 239-243  
 CODEN: PERKF9; ISSN: 1470-4358  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 IT 264913-39-5 264913-41-9  
 RL: PRP (Properties)  
 (heat of formation of diketopiperazines from the cyclization of dipeptides)  
 RN 264913-39-5 CAPLUS  
 CN Carbamic acid, [(2R,5S)-5-(hydroxymethyl)-3,6-dioxo-2-piperazinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



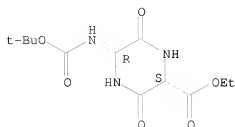
RN 264913-41-9 CAPLUS  
 CN Carbamic acid, [(2S,5S)-5-(hydroxymethyl)-3,6-dioxo-2-piperazinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 255869-53-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and conformation study of a diketopiperazine derivative as a possible  $\beta$ -turn mimic)  
 RN 255869-53-5 CAPLUS  
 CN 2-Piperazinecarboxylic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-3,6-dioxo-, ethyl ester, (2R,5S)-rel- (CA INDEX NAME)

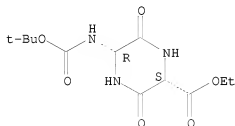
Relative stereochemistry.



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

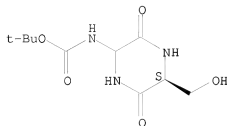
L7 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
 AB A symposium on the authors' preparation of  
 4-amino-3,5-dioxo-2-carboxypiperazine for use as a  $\beta$ -turn mimetic in  
 peptide chemical  
 AN 1999:578662 CAPLUS  
 DN 132:108257  
 TI A novel dioxopiperazine suitable as a  $\beta$ -turn constraint  
 AU Davies, J. S.; Stelmach-Diddams, M.; Fromentin, R.; Howells, A.; Cotton,  
 R.  
 CS Department of Chemistry, University of Wales, Swansea, SA2 8PP, UK  
 SO Peptide Science: Present and Future, Proceedings of the International  
 Peptide Symposium, 1st, Kyoto, Nov. 30-Dec. 5, 1997 (1999), Meeting Date  
 1997, 82-84. Editor(s): Shimonishi, Yasutsugu. Publisher: Kluwer,  
 Dordrecht, Neth.  
 CODEN: 68BYA5  
 DT Conference  
 LA English  
 IT 255869-53-5P 255870-05-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of from dipeptide as a  $\beta$ -turn constraint)  
 RN 255869-53-5 CAPLUS  
 CN 2-Piperazinecarboxylic acid, 5-[[[(1,1-dimethylethoxy)carbonyl]amino]-3,6-  
 dioxo-, ethyl ester, (2R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 255870-05-4 CAPLUS  
 CN Carbamic acid, [(5S)-5-(hydroxymethyl)-3,6-dioxo-2-piperazinyl]-,  
 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

AB Bicyclomycin (1) is a com. antibiotic whose primary site of action in *Escherichia coli* is the transcription termination factor rho. A recent structure-activity relationship study of 1 showed that replacing the C(6)-hydroxy group with alkoxy and thioalkoxy substituents led to dramatic losses of rho inhibitory activity in biochem. assays. The origin for this structural specificity has been explored by the synthesis and chemical, biochem., and biol. evaluation of C(6)-amino- (13), C(6)-(hydroxylamino)- (14), and C(6)-mercaptobicyclomycin (15). These compds., like 1, are capable of entering into hydrogen bond donor interactions with rho and are capable of undergoing C(6) ring opening to generate  $\alpha,\beta$ -unsatd. carbonyl, imine, or thione systems. The chemical reactivity of 13-15 was compared with that of 1. We observed that 1, upon treatment with EtSH under moderate and basic conditions, readily underwent C(6) hemiaminal bond cleavage followed by conjugate addition to  $\beta$ -methylene- $\alpha$ -ketoamide (2) to give Michael addition adducts whereas 13-15 reacted by initial cleavage of the C(1)-O(2) bond. Biochem. and biol. assays of 13-15 and related analogs demonstrated that the C(6) hydroxy group in 1 was essential for activity. We found that replacing the C(6)-hydroxy group in 1 with weaker hydrogen bond donors led to low inhibitory activities in the rho-dependent ATPase and transcription termination assays. None of the bicyclomycin derivs. exhibited antibiotic activity against *E. coli* W3350 cells at a 32 mg/mL concentration. The apparent specificity for the

C(6)-hydroxy group in 1 suggests that an efficient hydrogen bond donor interaction from the C(6)-hydroxy group to rho or the C(6) hemiaminal bond cleavage to 2 or both is necessary for drug function.

AN 1998:169757 CAPLUS

DN 128:239029

OREF 128:47145a,47148a

TI Role of the C(6)-Hydroxy Group in Bicyclomycin: Synthesis, Structure, and Chemical, Biochemical, and Biological Properties

AU Santillan, Alejandro, Jr.; Zhang, Xiangdong; Hardesty, Jon; Widger, William R.; Kohn, Harold

CS Departments of Chemistry and Biochemical and Biophysical Sciences, University of Houston, Houston, TX, 77204, USA

SO Journal of Medicinal Chemistry (1998), 41(7), 1185-1194

CODEN: JMCMAR; ISSN: 0022-2623

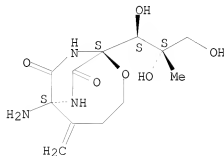
PB American Chemical Society

DT Journal

LA English

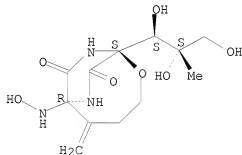
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 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis, structure, and properties of bicyclomycin analogs)  
 RN 205035-30-9 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-amino-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-, (1S,6S)-  
 (CA INDEX NAME)

Absolute stereochemistry.



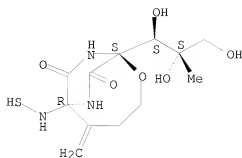
RN 205035-31-0 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-(hydroxyamino)-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-,  
 (1S,6R)- (CA INDEX NAME)

Absolute stereochemistry.



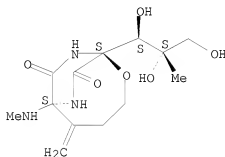
RN 205035-32-1 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-(mercaptoamino)-5-methylene-1-[(1,2,3-trihydroxy-2-methylpropyl)-,  
 [1S-[1α,1(1R\*,2R\*),6β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



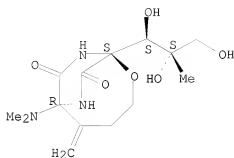
IT 205035-33-2P 205035-34-3P 205035-35-4P  
 205035-36-5P 205035-37-6P 205035-38-7P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (synthesis, structure, and properties of bicyclomycin analogs)  
 RN 205035-33-2 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-(methylamino)-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-,  
 (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 205035-34-3 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-(dimethylamino)-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-,  
 (1S,6R)- (CA INDEX NAME)

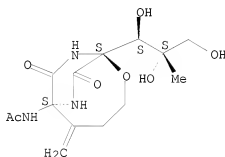
Absolute stereochemistry.



RN 205035-35-4 CAPLUS

CN Acetamide, N-[(1S,6S)-5-methylene-8,10-dioxo-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-2-oxa-7,9-diazabicyclo[4.2.2]dec-6-yl]- (CA INDEX NAME)

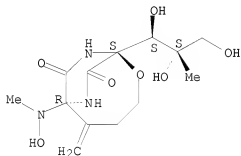
Absolute stereochemistry.



RN 205035-36-5 CAPLUS

CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione, 6-(hydroxymethylamino)-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-, (1S,6R)- (CA INDEX NAME)

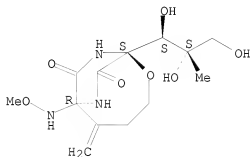
Absolute stereochemistry.



RN 205035-37-6 CAPLUS

CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione, 6-(methoxyamino)-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-, (1S,6R)- (CA INDEX NAME)

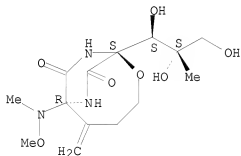
Absolute stereochemistry.



RN 205035-38-7 CAPLUS

CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
6-(methoxymethylamino)-5-methylene-1-[(1S,2S)-1,2,3-trihydroxy-2-methylpropyl]-, (1S,6R)- (CA INDEX NAME)

Absolute stereochemistry.



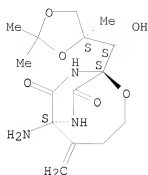
IT 205035-39-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(synthesis, structure, and properties of bicyclomycin analogs)

RN 205035-39-8 CAPLUS

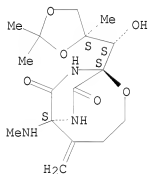
CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
6-amino-1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-5-methylene-, (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.



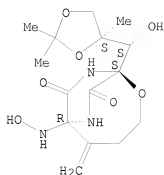
IT 205035-40-1P 205035-42-3P 205035-43-4P  
 205035-44-5P 205035-45-6P 205035-48-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (synthesis, structure, and properties of bicyclomycin analogs)  
 RN 205035-40-1 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-6-  
 (methylamino)-5-methylene-, (1S,6S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 205035-42-3 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-(hydroxyamino)-1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-  
 yl]methyl]-5-methylene-, (1S,6R)- (CA INDEX NAME)

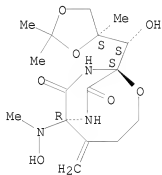
Absolute stereochemistry.



RN 205035-43-4 CAPLUS

CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
6-(hydroxymethylamino)-1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-5-methylene-, (1S,6R)- (CA INDEX NAME)

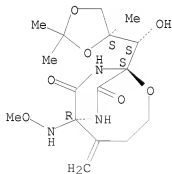
Absolute stereochemistry.



RN 205035-44-5 CAPLUS

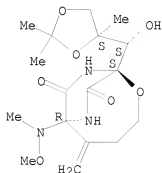
CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-6-(methoxyamino)-5-methylene-, (1S,6R)- (CA INDEX NAME)

Absolute stereochemistry.



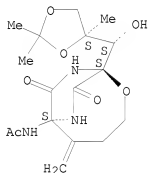
RN 205035-45-6 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-6-  
 (methoxymethylamino)-5-methylene-, (1S,6R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 205035-48-9 CAPLUS  
 CN Acetamide, N-[(1S,6S)-1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-5-methylene-8,10-dioxo-2-oxa-7,9-diazabicyclo[4.2.2]dec-6-yl]-  
 (CA INDEX NAME)

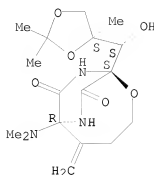
Absolute stereochemistry.



IT 205035-41-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis, structure, and properties of bicyclomycin analogs)

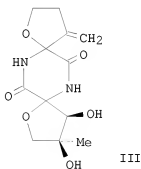
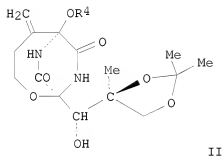
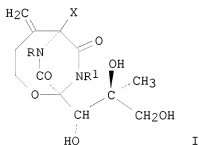
RN 205035-41-2 CAPLUS  
 CN 2-Oxa-7,9-diazabicyclo[4.2.2]decane-8,10-dione,  
 6-(dimethylamino)-1-[(S)-hydroxy[(4S)-2,2,4-trimethyl-1,3-dioxolan-4-yl]methyl]-5-methylene-, (1S,6R)- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN  
GI



AB Twelve bicyclomycin derivs. were synthesized to determine the effect of modification of the [4.2.2] bicyclic unit in bicyclomycin (I R = R1 = H, X = OH) on drug function. Few bicyclomycin derivs. have been described in which the [4.2.2] ring system has been modified. The compds. evaluated were divided into two categories: the two N-methyl-modified bicyclomycons (I; R = Me, R1 = H, Me) and the ten C(6)-substituted bicyclomycons (I; R =

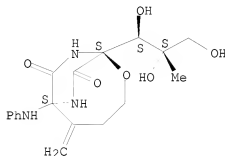
R1 = H, X = OMe, OEt, OCH<sub>2</sub>CF<sub>3</sub>, OCHMe<sub>2</sub>, OAc, OCOPh, SET, SPh, NHPH, H). Substituents introduced at the C(6) site included alkoxy, thioalkoxy, thiophenoxy, anilino, and hydrogen. A procedure was developed to synthesize select C(6)-substituted bicyclomycins. Bicyclomycin was first converted to bicyclomycin C(2'),C(3')-acetone (II; R<sub>2</sub> = H) and then treated with methanesulfonyl chloride to give in situ the corresponding C(6) mesylate II (R<sub>2</sub> = H). Treatment of II (R<sub>2</sub> = H) with the appropriate nucleophile followed by removal of the C(2'),C(3')-acetone group gave the desired C(6)-substituted bicyclomycin. The chemical properties of C(6) O-methylbicyclomycin (I; R = R<sub>1</sub> = H, X = OMe) were examined. Treatment of THF-H<sub>2</sub>O mixts. of I (R = R<sub>1</sub> = H, X = OMe) with excess EtSH maintained at "pH" 8.0-9.0 led to no detectable reaction, while at more basic "pH" values I (R = R<sub>1</sub> = H, X = OMe) underwent stereospecific conversion to the bis-spiro derivative III and no appreciable EtSH addition to the C(5)-C(5a) exomethylene unit. These results were compared to the reactivity of I (R = R<sub>1</sub> = H, X = OH) with EtSH. The stability (pH 7.4, 37 °C) of C(6)-substituted bicyclomycins I (R = R<sub>1</sub> = X = OMe, OCH<sub>2</sub>CF<sub>3</sub>, SET, SPh, NHPH, H) in aqueous solns. were examined. We observed that most of these compds. I (R = R<sub>1</sub> = X = OMe, SET, SPh, NHPH, H) underwent near complete change (>75%) within 200 h. The [4.2.2] bicyclic-modified bicyclomycins were evaluated in the rho-dependent ATPase assay and their antimicrobial activities determined using a filter disk assay. Most of the compds. were also tested in the transcription termination assay. The authors observed that all structural modifications conducted within the [4.2.2] bicyclic unit led to a loss of rho-dependent ATPase (I<sub>50</sub> > 400 μM) and to transcription termination (I<sub>50</sub> > 100 μM) inhibitory activities, as well as a loss of antimicrobial activity (MIC > 32 mg/mL). Only N(10)-methylbicyclomycin (I; R = Me, R<sub>1</sub> = H, X = OH) displayed moderate inhibitory activities in these assays. These findings indicated that the [4.2.2] bicyclic unit played an important role in the antibiotic-rho recognition process. Potential factors that govern this interaction are briefly discussed. The authors concluded that placement of an irreversible inactivating unit at the N- and O-sites within the [4.2.2] bicyclic unit in I (R = R<sub>1</sub> = H, X = OH) would likely prohibit the bicyclomycin derivative from efficiently binding to rho.

AN 1996:618959 CAPLUS  
 DN 126:6348h,6349a  
 OREF 126:6348h,6349a  
 TI Role of the [4.2.2] Bicyclic Unit in Bicyclomycin: Synthesis, Structure, Chemical, Biochemical, and Biological Properties  
 AU Santillan, Alejandro, Jr.; Park, Hyeung-geun; Zhang, Xiangdong; Lee, Oh-Seuk; Widger, William R.; Kohn, Harold  
 CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA  
 SO Journal of Organic Chemistry (1996), 61(22), 7756-7763  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PB American Chemical Society  
 DT Journal  
 LA English  
 IT 183374-30-3P  
 RL BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (synthesis, structure, chemical, biochem., and biol. properties of bicyclomycin derivs.)

RN 183374-30-3 CAPLUS

CN Bicyclomycin, 6-deoxy-6-(phenylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



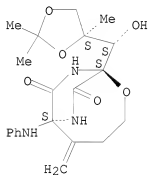
IT 183374-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(synthesis, structure, chemical, biochem., and biol. properties of  
bicyclomycin derivs.)

RN 183374-38-1 CAPLUS

CN Bicyclomycin, 6-deoxy-2',3'-O-(1-methylethylidene)-6-(phenylamino)- (9CI)  
(CA INDEX NAME)

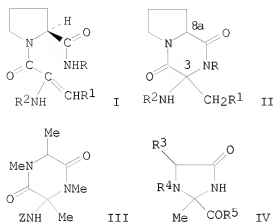
Absolute stereochemistry.



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

GI



AB Dehydropeptides I [R = Me, Ala-NHMe, R1 = H, R2 = PhCH2O2C (Z), Z-Ala; R = R1 = Me, R2 = Bz; R = Me, R1 = CHMe2, Ph, R2 = Ac; R = R1 = H, R2 = Z] were treated with 1,5-diazabicyclo[5.4.0]undec-5-ene (DBU) to give the corresponding pyrrolo[1,2-a]pyrazines II. Pyrazinedione III and imidazolidinone IV (R3 = H, R4 = Ac, R5 = piperidino) were prepared by cyclizing CH2:C(NHZ)CONMeCHMeCONHMe and Ac-Gly-NHC(:CH2)COR6 (R6 = piperidino), resp., with DBU, whereas IV (R3 = Me, R4 = H, R5 = Ala-NHMe) was prepared by treating Z-Ala-NHC(:CH2)CO-Ala-NHMe with DBU and then hydrogenating. The cyclization reaction involved an  $\alpha$ -addition of the amide to the acryloyl unit. The formation of a 6-membered ring was preferred over that of a 5-membered ring in the cyclization of the dehydropeptides. I (R = Me, R1 = H, R2 = Z) (V) was cyclized predominantly to the 3R,8aS-isomer of II with DBU treatment, whereas the 3R,8aR-isomer of II was the predominant product resulting from the treatment of V with NaOH. Stereoselective ring closure was also observed for other dehydropeptides. The dehydroalanine-containing peptides were prepared by removal of HMe from the corresponding S-methylcysteine-containing peptides.

AN 1977:439832 CAPLUS

DN 87:39832

OREF 87:6303a,6306a

TI Amino acids and peptides, XVII. Dehydroamino acids, IV. Ring closure of dehydropeptides

AU Oehler, Elisabeth; Schmidt, Ulrich

CS Org.-Chem. Inst., Univ. Wien, Vienna, Austria

SO Chemische Berichte (1977), 110(3), 921-41

CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

IT 63095-86-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 63095-86-3 CAPLUS

CN Carbamic acid, (1,2,4,5-tetramethyl-3,6-dioxo-2-piperazinyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

